

A PARALLEL AND ADAPTIVE MULTIGRID SOLVER FOR THE SOLUTIONS OF THE OPTIMAL CONTROL OF GEOMETRIC EVOLUTION LAWS IN TWO AND THREE DIMENSIONS

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SUMMARY

We present a problem concerning the optimal control of geometric evolution laws. This is a minimisation problem that aims to find a control η which minimises the objective functional J subject to some imposed constraints. We apply this methodology to an application of whole cell tracking. Given two sets of data of cell morphologies, we may solve the optimal control problem to dynamically reconstruct the cell movements between the time frame of these two sets of data. This problem is solved in two and three space dimensions, using a state-of-the-art numerical method, namely multigrid, with adaptivity and parallelism.

Key words: *Optimal control, geometric evolution laws, phase-field, multigrid, parallel, mesh adaptivity, cell tracking*

1 INTRODUCTION

Optimal control was initialised more than half a century ago, and since then it has been successfully applied to solve different types of problems [1]. Recently, Blazakis et al. in [2] considered an optimal control problem of geometric evolution laws with semi-linear partial differential equations (PDEs) that is based upon the work of Haußer et al. [3].

To generally outline the model, given two sets of data, one is the initial data (denoted $\phi^{t=0}$), and the second data is observed at a later time (denoted ϕ_{obs}), the optimal control problem aims to find a space-time distributed forcing $\eta : \Omega \times [0, T] \rightarrow \mathcal{R}$ which minimises an objective functional J :

$$\min_{\eta} J(\phi, \eta), \quad \text{with } J \text{ given by Equation (2),} \quad (1)$$

$$J(\phi, \eta) = \frac{1}{2} \int_{\Omega} (\phi(t = T) - \phi_{\text{obs}})^2 + \frac{\theta}{2} \int_0^T \int_{\Omega} \eta^2, \quad (2)$$

where Ω is a fixed spatial domain which is assumed to be large enough to contain both known sets of data and linear trajectories of the evolution between the two, $\theta > 0$ is a regularisation parameter, $[0, T]$ is the temporal domain, T is the end time. Physically, η describes the evolution laws of the positions of the computed data matching closely to the observed data at the final time T . The first term of the right-hand side of Equation (2) is the so called fidelity term which measures the distance between the approximated solution of the model and the target data ϕ_{obs} ; the second term is the regularisation which is necessary to ensure a well-posed problem [1].

The ϕ in Equations (1) and (2) are subject to the constraints imposed from the geometric evolution laws, such as the Allen-Cahn equation which takes the following form,

$$\epsilon \frac{\partial \phi}{\partial t} = \epsilon \Delta \phi - \frac{G'(\phi)}{\epsilon} + c_G \eta + \lambda, \quad (3)$$

where $\phi(x, y, z, t)$ is the phase-field variable, ϵ is the thickness of the diffuse interface determined by ϕ , $G(\phi) = \frac{1}{4}(1 - \phi^2)^2$ is a double well potential which has minima at ± 1 , $c_G = \frac{1}{\sqrt{2}} \int_{-1}^1 G(r)^{\frac{1}{2}} dr$

is a scaling constant that depends on the double well potential and $\lambda(t)$ is a time-dependent volume constraint [4]. This $\lambda(t)$ on the enclosed volume from our phase-field approach is given by a constraint on the mass and the linear interpolant of the mass of the initial and target diffuse interface data is defined as

$$M_\phi(t) = \int_{\Omega} \phi^{t=0} + \frac{t}{T}(\phi_{\text{obs}} - \phi^{t=0}). \quad (4)$$

This volume constraint $\lambda(t)$ is determined along with Equation (3) such that

$$\int_{\Omega} \phi(t) = M_\phi(t). \quad (5)$$

As the thickness of interface $\epsilon \rightarrow 0$, conservation of mass yields volume conservation.

For effective computation of the derivative of the objective functional J , we include the adjoint state $p(x, y, z, t)$, which is defined as

$$\frac{\partial p}{\partial t} = -\Delta p + \frac{G''(\phi)}{\epsilon} p. \quad (6)$$

We further assume the domain boundaries $\partial\Omega$ are away from the specified data, and thus have no effect on the evolution. The conditions on the boundaries for ϕ and p are $\frac{\partial \phi}{\partial \mathbf{v}} = \frac{\partial p}{\partial \mathbf{v}} = 0$ on $\partial\Omega$, where \mathbf{v} denotes the outward-pointing normal to the boundary $\partial\Omega$. Note the control η has no boundary conditions as it is only valid within the interior of the domain Ω .

2 METHODOLOGY

The control η is updated and obtained through an iterative approach, where the Allen-Cahn and adjoint Equations (3) and (6) in the fixed time frame $[0, T]$ have to be solved repeatedly. The described optimal control problem may require an enormous amount of computation. To obtain a numerical approximation of the solution of this optimal problem is non-trivial, and additional challenges arise, such as memory requirement (since solutions of ϕ , p and η from every time step are required to be stored), when pursuing accuracy, i.e. ϵ tends to 0, as well as simulations in 3-D.

The software that we used here, Campfire v2.0, is dependent upon an open source software library, namely PARAMESH [5]. This library generates structured, cell-centred, Cartesian meshes and provides hierarchical mesh adaptivity in parallel in two and three dimensions. Our software tool, Campfire (original version), has been successfully applied to a number of different applications, such as binary alloy solidification [6]. The core numerical method implemented in this tool is the multigrid algorithm with the full approximation scheme and multi-level adaptive technique (MLAT) [7]. The former extends the multigrid algorithm to deal with nonlinear problems, and the latter enables the use of adaptive meshes. The parallelization is through domain decomposition, and a dynamic load-balancing approach is taken which allows meshes to adapt dynamically based upon the solution.

In the optimal control problem, both Equations (3) and (6) are discretized fully-implicitly using a second-order backward differential formula (BDF2). At each implicit time step, the ordinary differential equations (ODEs) are then discretized spatially using a second-order finite difference method (FDM) with a five- or seven-point stencil in 2-D or 3-D, respectively. The resulting algebraic systems arising at each implicit time step are then solved by the nonlinear multigrid with FAS.

Due to this nature of the problem, we implemented a robust in-house multigrid algorithm with two different depths of the standard V-cycle strategy. That is, solving the Allen-Cahn equation in a grid hierarchy where its finest grid has sufficient grid points for the chosen ϵ ; the backward adjoint equation is then solved using only part of the grid hierarchy to improve the efficiency.

The application chosen for this optimal control problem is whole cell tracking, which will in turn help to understand cell migration. In this application, the given data includes cell morphologies. The initial data describes the known position and morphologies of cells at $t = 0$ and the second set of data illustrates the position and morphologies of these cells at the final time $t = T$.

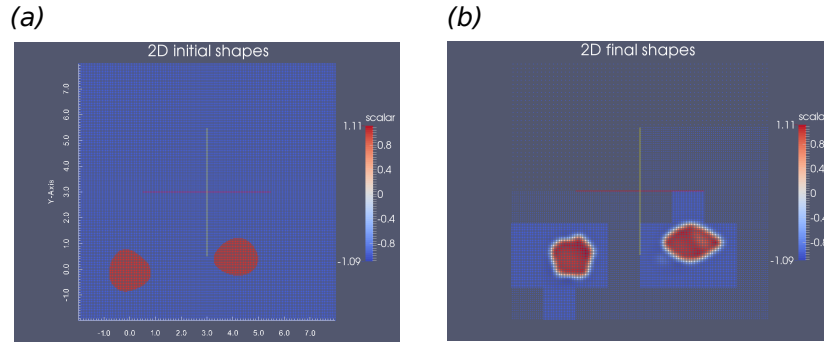


Figure 1: (a) The initial shapes; (b) the computed final shape.

3 RESULTS AND CONCLUSIONS

In this abstract, we include two sets of results. Firstly, we take an example from [2], which figures two 2-D cells on a domain $\Omega = [-2, 8] \times [-2, 8]$. The initial shapes and the computed results are shown in Figure 1 (a) and (b) respectively. The evolution of the objective function J is illustrated in Figure 3.

We also present a single-cell 3-D simulation. The initial and final shapes are presented in Figure 2. This simulation is generated using high performance computing cluster provided by the University of Sussex and within the adaptive meshes used, the finest mesh if refined everywhere has a resolution of 256^3 . The presented η is computed after 108 iterations, and the values of the objective function J are illustrated in Figure 3, where it is converged to a small but positive, non-zero value, as expected.

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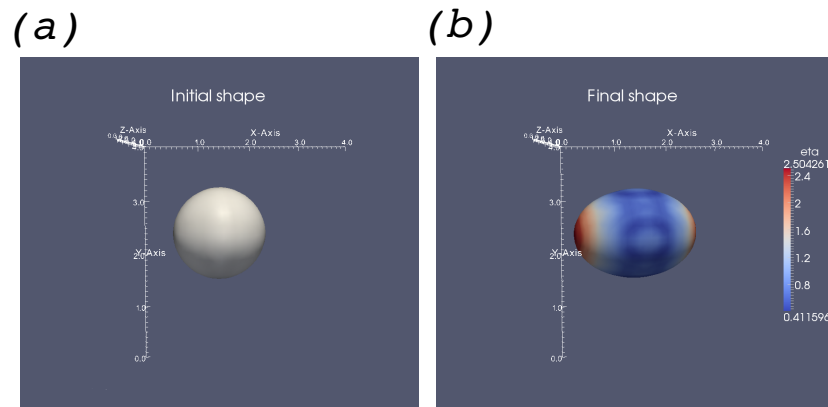


Figure 2: (a) The isosurface of $\phi = 0$ of the initial shape; (b) the isosurface of the computed final shape, we present the solution of η as colours on the isosurface.

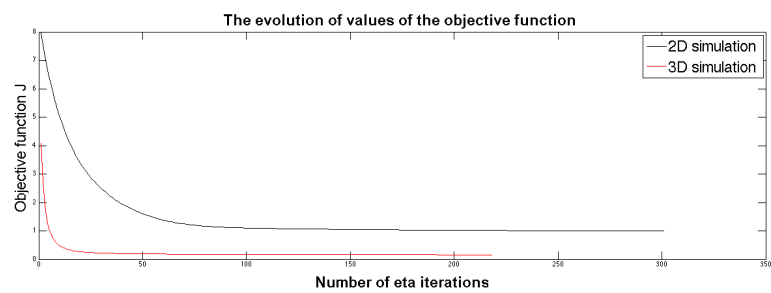


Figure 3: The evolution of values of η .